High Temperature Enthalpy of Lutetium Trifluoride

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The rare-earth fluorides (REFs) are used in chemistry, optics, and microelectronics. Unfortunately caloric properties of rare-earth fluorides have not been reliably investigated. There is only one work [1] in which the direct measurements of LuF_3 high temperature enthalpy were carried out.

The aim of this work was to investigate the enthalpy and the heat capacity of LuF_3 over a wide temperature range. This includes both solid and liquid states and the solid-solid phase transition and melting-crystallization regions. The LuF_3 was synthesized from metallic, high purity Lu. LuF_3 was refined from LuOF and Lu_2O_3 by way of vacuum distilling. The LuF_3 enthalpy was measured in a high-temperature massive isoperibol drop calorimeter from 392 to 1597 K. The temperature of the sample was measured by the W-Re thermocouple. The thermocouple was calibrated at the melting points of pure Sn, Al, Cu and Ni. The error of the enthalpy measurements was determined in experiments with the reference substance α-Al_2O_3. It did not exceed 0.3%. The data in the single-phase regions were fitted by the least squares method. For the phase of β - YF_3 type, the equation using the contributions by lattice vibrations and by vacancies was used. It was determined that the vacancy term is statistically negligible and the anharmonic vibrational term was proportional to the fourth degree of the temperature. The θ_D value was estimated. The values of heat capacity obtained by extrapolation of this equation to the room temperature are in excellent agreement with data [2]. The enthalpies of solid-solid phase transition and melting from [1] coincides with our value within the limit of experimental error. The heat capacity change on solid-solid phase transition and those on melting differ from [1] in sign.

[1] F.H. Spedding and D.C. Henderson, *J. Chem. Phys.* **54**, 2476 (1971).
[2] H.E. Flotow and P.A.G. O'Hare, *J. Chem. Phys*. **74** 3046 (1981).